1,3-Benzodioxole-5-methanol

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 7.40

Global applicability domain: Inside

Local applicability domain index: 6.57e-01

Confidence level: 4.20e-01

Nearest Neighbors from the Training Set

Image not found
Methylparaben
Measured: 8.57
Predicted: 7.06

Image not found
1-Octanol
Measured: 6.03
Predicted: 5.95

Image not found
Phenacetin
Measured: 9.59
Predicted: 9.23

Image not found
Cyclohexanol
Measured: 5.18
Predicted: 4.72

Image not found
1-Hexanol
Measured: 5.18
Predicted: 4.67